

Niridazole
61-57-4 | DTXSID6045244

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.30e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.37e-01

Confidence level: 5.58e-01

Nearest Neighbors from the Training Set

Image not found

Niridazole

Measured: 6.07e-04

Predicted: 6.30e-03

Image not found

S-[2-Oxo-2-(phenylamino)ethyl]
thiocarbamate

Measured: 4.76e-02

Predicted: 6.62e-02

Image not found

Nithiazide

Measured: 1.39e-03

Predicted: 3.99e-02

Image not found

Guanidine, (2-benzothiazolyl)-

Measured: 3.62e-03

Predicted: 2.64e-03

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Dimethoate

Measured: 1.09e-01

Predicted: 1.03e-01